METHODOLOGY for DETERMINING CHEMICAL AND PHYSICAL PROPERTIES, FACTOR VALUES AND SCREENING CONCENTRATION BENCHMARKS

FOR VOLATILE SUBSTANCES LISTED IN THE U.S. EPA's SUPERFUND CHEMICAL DATA MATRIX (SCDM)

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ACRONYMS and ABBREVIATIONS

AALAC	Ambient Aquatic Life Advisory Concentrations
ACGIH	American Conference of Governmental Industrial Hygienists
ASTSDR	Agency for Toxic Substances and Disease Registry
AWQC	Ambient Water Quality Criteria
BCF	Bioconcentration Factor
CAS RN	Chemical Abstracts Survey Registration Number
CCC	Criteria Continuous Concentration
CFR	Code of Federal Regulations
CMC	Criteria Maximum Concentration
EPA	United States Environmental Protection Agency
EPI	Estimation Programs Interface
FDAAL	Food and Drug Administration Action Levels
f_s	Sorbent Content (fraction of clays plus organic carbon)
HEAST	Health Effects Assessment Summary Tables
HEDR	Handbook of Environmental Degradation Rates
HRS	Hazard Ranking System
HTF	Human Toxicity Factor
IUR	Inhalation Unit Risk
IRIS	Integrated Risk Information System
K_d	Soil/Water Distribution Coefficient
K_{oc}	Soil Organic/Carbon Partition Coefficient
LC	Lethal Concentration
LD	Lethal Dose
Log K_{ow}	Logarithm of the n-Octanol-Water Partition Coefficient
MCI	Molecular Connectivity Index
MCLs	Maximum Contaminant Levels
MCLGs	Maximum Contaminant Level Goals
MRL	Minimal Risk Level
MW	Molecular Weight
NAAQS	National Ambient Air Quality Standards
NESHAPs	National Emission Standards for Hazardous Air Pollutants
NIOSH	National Institute for Occupational Safety and Health
PPRTV	Provisional Peer Reviewed Toxicity Values
REL	Reference Exposure Level
RfC	Reference Concentration
RfD	Reference Dose
RME	Reasonable Maximum Exposure
RSL	Regional Screening Level
RTECS	Registry of Toxic Effects of Chemical Substances
RTI	Research Triangle Institute
SCDM	Superfund Chemical Data Matrix
SF	Slope Factor (Cancer)
SRC	Syracuse Research Corporation
WOE	Weight-of-Evidence

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1.0 INTRODUCTION

This appendix contains information regarding procedures for determining chemical and physical properties, factor values and screening concentration benchmarks for the subset of Superfund Chemical Data Matrix (SCDM) substances listed below. The factor values and benchmarks for this set of SCDM substances supersede any previous values beginning April 1, 2012. These new values and benchmarks reflect the EPA's revised methodology for determining risk, as described in the EPA's *Risk Assessment Guidance for Superfund (RAGS) Volume 1: Human Health Evaluation Manual, Part F: Supplemental Guidance for Inhalation Risk Assessment* (EPA-540-R-070-002/OSWER 9285.7-82) and Soil Screening Guidance: Technical Background Document (EPA/540/R95/128). Only SCDM substances that are identified as volatile based on associated Henry's Law Constants ≥ $1x10^{-5}$ atm·m^3/mol and molecular weights < 200 g/mol (*Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites*, http://www.epa.gov/superfund/health/conmedia/soil/pdfs/ssg_main.pdf), were selected for this determination. The 49 substances identified as volatile are listed in Table 1.

Table 1. Substances Listed in SCDM and Identified as Volatile

Acenaphthene	Dichloroethane, 1,2-	Pyrene
Acetone	Dichloroethylene, 1,2-	Styrene
Acrolein	Dichloroethylene, 1,2-(*mixed isomers*)	Tetrachloroethane, 1,1,2,2-
Anthracene		Tetrachloroethylene
Benzene	Dichloroethylene, 1,2-cis-	Toluene
Bromodichloromethane	Dichloroethylene, 1,2-trans-	Trichlorobenzene, 1,2,4-
Carbon disulfide	Dichloropropane, 1,2-	Trichloroethane, 1,1,1-
Carbon tetrachloride	Dichloropropene, 1,3-	Trichloroethane, 1,1,2-
Chlorobenzene	Ethylbenzene	Trichloroethylene
Chloroform	Fluorene	Trichlorofluoromethane
Cumene	Mercury (elemental)	Trichloropropane, 1,2,3-
Dibenzofuran	Methyl ethyl ketone (2-butanone)	Vinyl acetate
Dibromo-3-chloropropane, 1,2-	Methyl tert-butyl ether	Vinyl chloride
Dibromoethane, 1,2-	Methylene chloride	Xylene, p-
Dichlorobenzene, 1,4-	Nitrobenzene	Xylene, m-
Dichloroethane, 1,1-	Methylnaphthalene, 2-	Xylene, o-
	Naphthalene	Xylenes

2.0 DATA SELECTION METHODOLOGY

This section describes the methodology used for collecting and selecting data to determine factor values and screening concentration benchmarks for forty nine volatile substances listed in SCDM (see Section 1.0 of this methodology document). It also specifies data source hierarchies and how the hierarchies are applied for each data type collected.

2.1 Hazardous Substance Identities and General SCDM Protocols

Compiling data for SCDM requires determining which data reasonably apply to a hazardous substance. In some cases, data in the references cited in Sections 2.2 through 2.7 are available for only classes and mixtures of hazardous substances and not for the individual substances that make up that mixture. In general, if any member of these classes is present at a hazardous waste site, it is assumed that the most toxic, most persistent, or most bioaccumulative member of the class is present. In other words, from among the data given in the specified references for members of these classes, SCDM contains those data resulting in the greatest Hazardous Ranking System (HRS) factor values as specified by the HRS (e.g., lowest Reference Dose [RfD], highest cancer slope factor, longest half-life, greatest bioaccumulation factor).

2.1.1 Generic Values

Of the 49 volatile substances listed in Section 1.0, SCDM contains generic values for one individual substance:

- For mercury (both elemental and inorganic species), the inhalation RfD is calculated using the Reference Concentration (RfC) for elemental mercury vapor. The vapor pressure, Henry's Law Constant, and distribution coefficient are for elemental mercury.

- Generic RfD and RfC values are obtained for xylenes, to represent values used for p-xylene, m-xylene, and o-xylene, and xylenes.

2.1.2 Compound Classes with Values for Individual Substances

Of the 49 volatile substances listed in SCDM (see Section 1.0), SCDM contains individual values for three substances that are included in one compound class:

- For xylenes, values are provided for o-xylene, m-xylene, and p-xylene. If no data can be found in the specified references for the individual substances but data are available for the generic class of xylenes, SCDM assigns the generic value to the individual substances. The class of xylenes is a relatively small set of isomers, that are likely to occur as mixtures. The class also is well defined in that the generic class (e.g., xylenes) almost always refers to a mixture of all members of the class (o-, m-, and p-xylene). The expected similarity in chemical behavior for members of each class, as well as the likelihood that they will occur as mixtures, makes using data from mixtures reasonable.

2.1.3 Substitution Classes

In some cases, SCDM data for a particular substance may be substituted from a parent substance class. SCDM contains three major classes of data for which data substitution may be applied: (1) toxicity, (2) ground water mobility, and (3) other. A parent Chemical Abstracts Survey Registration Number (CAS RN) can be entered for any of these three substitution classes and, in this case, SCDM uses the relevant data from the parent substance for the substance of interest. For substitutions of toxicity data, all toxicity and benchmark data used to determine human- or eco-toxicity factor values can be substituted. Ground water mobility class data substitutions include water solubility, geometric mean water solubility and soil/water distribution coefficient (K_d). Parent class data also may be substituted for hydrolysis, biodegradation, photolysis, and volatilization half-lives, as well as bioconcentration factor (BCF) and logarithm of the n-octanol-water partition coefficient (Log K_{ow}).

Currently in SCDM, two groups of substances inherit data from a parent substance: metals and radioactive substances. Generally, metal-containing substances inherit data for ground water mobility values with the elemental metal as the class parent. Radioactive isotopes may inherit data from the primary radioactive element.

2.2 Data Used to Determine Human Toxicity Factor Values

Section 2.2 details how data are obtained and used for determining human toxicity factor (HTF) values. RfD, RfC, cancer slope factor (SF) and inhalation unit risk (IUR) values are identified and used to determine the HTF value for each substance. These values also are used to determine exposure pathway screening concentration benchmarks (see Section 3.0 of this methodology document).

For purposes of assigning the HTFs, data for RfD, RfC, IUR, and cancer slope factor values are identified for each substance according to a hierarchy of references. Of the values selected, the most conservative (i.e., most protective of human health) is used to determine the HTF, regardless of exposure route or whether the value represents a non-cancer or cancer effect. The following exceptions are applied to this approach:

(1) the RfD_{oral} that is available for elemental mercury (Reference Exposure Limit from the California Environmental Protection Agency) is currently being re-evaluated for use in determining Regional Screening Levels (RSLs) and is not used in SCDM, and

(2) generic RfD and RfC values are obtained for xylenes, to represent values used for p-xylene, m-xylene, and o-xylene, and xylenes.

Data values were obtained from the following references, listed in order of preference:

- U.S. EPA. 2011. *Integrated Risk Information System (IRIS)*. Office of Research and Development, Cincinnati, OH. http://www.epa.gov/iris. Accessed February 2012.

- The Provisional Peer Reviewed Toxicity Values (PPRTVs) derived by the EPA's Superfund Health Risk Technical Support Center (STSC) for the EPA Superfund program. http://hhpprtv.ornl.gov. Accessed February 2012.

- The Agency for Toxic Substances and Disease Registry (ATSDR) minimal risk levels (MRLs). http://www.atsdr.cdc.gov/mrls/mrllist.asp. Accessed February 2012.

- The California Environmental Protection Agency (OEHHA) Office of Environmental Health Hazard Assessment's Chronic Reference Exposure Levels (RELS) and Cancer Potency Values. Main database. http://oehha.ca.gov/risk/chemicalDB/index.asp. Accessed February 2012.

- PPRTV appendix screening toxicity values. http://hhpprtv.ornl.gov/quickview/pprtv_compare.php. Accessed February 2012.

- U.S. EPA. 2003. *Health Effects Assessment Summary Tables (HEAST): Summary of HEAST Values*. Office of Research and Development/Office of Emergency and Remedial Response, Washington, DC. http://epa-heast.ornl.gov/. Accessed February 2012.

2.2.1 Non-Carcinogenic Toxicity Values

2.2.1.1 Reference Dose (RfD), Oral; Reference Concentration (RfC), Inhalation

SCDM contains RfD values for oral toxicity and RfC values for inhalation toxicity that are used for determining HTF values. RfC values are converted from concentrations into inhalation dosages or RfD_{inhal} values for determining HTF values using the following equation:

$$RfD_{inhal} = \frac{RfC \times IR \times AR}{BW \times 100}$$

Where:
RfD_{inhal} = Reference Dose in Air (mg/kg-day)
RfC = Reference Concentration in Air (mg/m^3)
IR = Inhalation Rate (20 m^3/day)
AR = Absorption (100 assumed unless otherwise specified by source), unitless
BW = Adult Body Weight (70 kg)

Using the exposure assumptions listed above, the equation may be simplified as:

$$RfD_{inhal}(mg/kg-day) = RfC_{inhal} \times AR \times 2.857 \times 10^{-3}$$

Equation (2) is used to convert RfCs to inhalation RfDs. The resulting RfD_{inhal} values are used to determine HTF values. If the reference source used to provide the RfD or RfC does not provide a corresponding absorption, it is assumed to be 100.

2.2.1.2 LD_{50} – Oral, Dermal; LC_{50} - Inhalation

When a reference dose or cancer slope factor with weight-of-evidence is not available, SCDM uses the LD_{50} (oral, dermal) or LC_{50} (inhalation) to assign human toxicity factor values. The lowest of the two values is selected. These values are not used to calculate benchmarks. The reference hierarchy used is listed below, in order of priority:

- American Conference of Governmental Industrial Hygienists (ACGIH). 2012. Threshold Limit Values and Biological Exposure Indices, ACGIH, Cincinnati, OH.ISBN: 978-1-607260-48-6. http://www.acgih.org/store/ProductDetail.cfm?id=2190.

- National Institute for Occupational Safety and Health (NIOSH). 2011. Registry of Toxic Effects of Chemical Substances (RTECS). http://www.cdc.gov/niosh/rtecs/.

- U.S. National Library of Medicine Toxicology Data Network (TOXNET) ChemIDPlus. 2011. National Institutes of Health, Health & Human Services. Rockville, MD. http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?CHEM.

- C-E Environmental, Inc. 1990. The Identification of Health Effects Data for Chemicals Contained in the Clean Air Act Amendments: Final Report to Dr. John Vanderbury. U.S. Environmental Protection Agency, Research Triangle Park, NC.

LD_{50} and LC_{50} values were not needed to assess HTF values and, therefore, were not collected for the 49 volatile substances listed in Section 1.0 of this methodology document.

2.2.2 Carcinogenic Toxicity Values

The cancer slope factors (SF) and weight-of-evidence (WOE) classifications in this section are used to determine the HTF values for carcinogenic substances.

2.2.2.1 Weight-of-Evidence (WOE) – Oral, Inhalation

The carcinogenic risk WOE classification from the same reference that provided the corresponding cancer risk value (e.g., IUR or SF) is used for each substance. If only an oral WOE classification is provided for substances identified as carcinogenic via inhalation, it is recorded for the inhalation cancer risk value. In some instances, two or more WOE assessments are discussed in a single reference. In these cases, the WOE assessment that is associated with the data value is used, which is typically the most recent assessment.

The EPA 2005 guidelines present the following five categories for WOE:

- Carcinogenic to Humans
- Likely to Be Carcinogenic to Humans
- Suggestive Evidence of Carcinogenic Potential
- Inadequate Information to Assess Carcinogenic Potential
- Not Likely to Be Carcinogenic to Humans

WOE classifications are collected for a substance's cancer risk value, and final WOE category letters (A, B, C) are assigned based on the EPA's 2005 WOE classifications approach and values presented in Table 2. Final WOE category letters are then used to determine HTFs (see HRS Section 2.4.1.1, Table 2-4 [40 CFR Part 300]).

Table 2. SCDM Weight-of-Evidence (WOE) Assignment

SCDM WOE Classifications	2005 WOE Descriptors
A	Carcinogenic to Humans
B	Likely to be Carcinogenic
C	Suggestive Evidence of Carcinogenic Potential

2.2.2.2 Cancer Slope Factor (SF) – Oral; Inhalation Unit Risk (IUR)

SCDM contains SF values for oral toxicity and IUR values for inhalation toxicity. IUR values are converted into inhalation SF (SF_{inhal}) values for use in determining HTF values.

IURs were converted to inhalation cancer slope factors using the following equation:

$$SF_{inhal} = \frac{IUR \times BW \times CF \times 100}{IR \times AR}$$

Where:
SF_{inhal} = Cancer Slope Factor $(mg/kg\text{-}day)^{-1}$
IUR = Inhalation Unit Risk $(\mu g/m^3)^{-1}$
BW = Adult Body Weight (70 kg)
CF = Conversion Factor (1,000 µg/mg)

IR = Inhalation Rate (20 m^3/day)
AR = Absorption (100 assumed unless otherwise specified)

Using the exposure assumptions listed above, this equation can be simplified as:

$$SF_{inhal}(mg/kg-day)^{-1} = \frac{IUR \times 3.50 \times 10^5}{AR}$$

Equation (4) is used to convert the IUR value to an inhalation cancer SF, and the resulting inhalation cancer SF is evaluated with a corresponding WOE (see Section 2.2.2.1 above) to assign an HTF value based on HRS Table 2-4 (40 CFR Part 300). If the reference source used did not provide absorption, it is assumed to be 100.

2.3 Mobility Information

Vapor pressure and Henry's Law Constant are used to determine the gas migration potential and gas mobility potential. Water solubility and the soil/water distribution coefficient are used to determine the ground water mobility factor. Henry's Law Constant is also used to determine volatilization half life.

2.3.1 Vapor Pressure

SCDM uses data from the following references to obtain vapor pressures, listed in order of preference:

- PHYSPROP Database. 2010. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.syrres.com/what-we-do/databaseforms.aspx?id=386. Accessed February 2012.

- The Estimation Programs Interface (EPI) Suite™ (experimental values). Developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/opptintr/exposure/pubs/episuite.htm. Accessed February 2012.

- Perry's Chemical Engineers' Handbook, 8th Edition. 2008, Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

- CRC Handbook of Chemistry and Physics, 92nd Edition. June 2011. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.

- O'neil, M., and A. Smith (Eds). 2012. The Merck Index, 14th Edition. Merck & Co., Inc., Rahway, NJ.

- Estimation procedures set forth by Lyman *et al*. 1990. Handbook of Chemical Property Estimation Methods. American Chemical Society, Washington, DC, as described in Research Triangle Institute (RTI). 1996. Chemical Properties for SCDM Development, Prepared for U.S. EPA Office of Emergency and Remedial Response.

If a recommended value is not available, SCDM uses a value measured at 25°C. If more than one value measured at 25°C is available, SCDM uses the highest one. If no value is available at 25°C, the value determined at a temperature closest to 25°C is selected. If more than one value measured at the same temperature is available and none is recommended, SCDM uses the highest value. If no temperature is specified for all vapor pressure measurements for a substance, SCDM uses the highest value.

If vapor pressure values are not available in PHYSPROP, they are taken from EPI Suite™ experimental values. If not available in EPI Suite™, values are taken from the subsequent references listed above, in the order they are listed. If no vapor pressure values are available in any of the first five references listed, or if the referenced value is suspect, a value may be either selected from a data source outside the hierarchy or estimated. For any given substance, suspect values are identified by comparison with other vapor pressure values in SCDM data sources or other sources of chemical property data. The procedures described in Lyman *et al*. (1990) are used to estimate vapor pressure. RTI (1996) describes the use of these procedures for specific hazardous substances.

For nonmetallic substances, if a vapor pressure is not available, a normal boiling point is obtained from the CRC Handbook of Chemistry and Physics. If a boiling point is not available from the CRC Handbook, a value is obtained from The Merck Index. If the boiling point at 1 atmosphere (atm) is <25°C, a default vapor pressure of 760 Torr is used with the assumption that the substance is a gas at 25°C.

If no vapor pressure is available for a substance and the normal boiling point is ≥25°C, SCDM assumes that the substance is in a particulate form, rather than a gaseous form, and no vapor pressure is assigned. This assumption is made because the absence of a vapor pressure value often reflects an extremely low and difficult to measure (under standard conditions) value for nongaseous substances.

For the 49 volatile substances listed in Section 1.0 of this methodology document, only the PHYSPROP database was needed to obtain vapor pressure values.

2.3.2 Henry's Law Constant

SCDM uses data from the following references for Henry's Law Constants, listed in order of preference:

- PHYSPROP Database. 2010. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.syrres.com/what-we-do/databaseforms.aspx?id=386. Accessed February 2012.

- The Estimation Programs Interface (EPI) Suite™ (experimental values). Developed by the US Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/opptintr/exposure/pubs/episuite.htm. Accessed February 2012.

- Yaws' Handbook of Thermodynamic and Physical Properties of Chemical Compounds. Knovel. http://www.knovel.com.

- CHEMFATE Database. 2008. Syracuse Research Corporation (SRC). Syracuse, NY http://www.srcinc.com/what-we-do/databaseforms.aspx?id=381.

- Estimation procedures set forth by Lyman *et al*. 1990. Handbook of Chemical Property Estimation Methods. American Chemical Society, Washington, DC, as described in Research Triangle Institute (RTI). 1996. Chemical Properties for SCDM Development, Prepared for U.S. EPA Office of Emergency and Remedial Response.

If a recommended value is not available, SCDM uses a value measured at 25°C. If more than one value measured at 25°C is available, SCDM uses the highest one. If no value is available at 25°C, the value determined at a temperature closest to 25°C is selected. If more than one value measured at the same temperature is available and none is recommended, SCDM uses the highest value. If no temperature is specified for all Henry's Law Constants for a substance, SCDM uses the highest value.

If a Henry's Law constant is not available in PHYSPROP, values are obtained from the references listed above in the order listed. If no Henry's Law Constant is available from the first four references or if the values provided are suspect, procedures described in Lyman *et al*. (1990) are used to estimate a Henry's Law constant. For the 49 volatile substances listed in Section 1.0 of this methodology document, only the PHYSPROP database was needed to obtain Henry's Law constants.

2.3.3 Water Solubility

Water solubility values are used, along with distribution coefficient (K_d) values, to calculate the ground water mobility of hazardous substances that do not meet observed release criteria. All hazardous substances that are available to migrate from sources at a site to the ground water are evaluated for ground water mobility. Water solubility values are also used to assign a bioaccumulation potential factor value for hazardous substances when BCF data or logarithm of the n-octanol-water partition coefficient (Log K_{ow}) data are not available.

2.3.3.1 Water Solubility - Nonmetallic Compounds

SCDM obtains water solubility values for nonmetallic volatile substances from the following references, listed in order of priority:

- PHYSPROP Database. 2010. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.syrres.com/what-we-do/databaseforms.aspx?id=386. Accessed February 2012.

- The Estimation Programs Interface (EPI) Suite™ (experimental values) developed by the US Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/opptintr/exposure/pubs/episuite.htm. Accessed February 2012.

- CRC Handbook of Chemistry and Physics, 92nd Edition. June 2011. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.

- Perry's Chemical Engineers' Handbook, 8th Edition. 2008, Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

- Lange's Handbook of Chemistry. 16th Edition. 2004, Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.

- Yaws' Handbook of Thermodynamic and Physical Properties of Chemical Compounds. Knovel. http://www.knovel.com.

- Estimation procedures set forth by Lyman *et al*. 1990. Handbook of Chemical Property Estimation Methods. American Chemical Society, Washington, DC, as described in Research Triangle Institute (RTI). 1996. Chemical Properties for SCDM Development, Prepared for U.S. EPA Office of Emergency and Remedial Response.

If a recommended value is not available, SCDM uses a value measured at 25°C. If more than one value measured at 25°C is available, SCDM uses the highest one. If no value is available at 25°C, the value determined at a temperature closest to 25°C is selected. If more than one value measured at the same temperature is available and none is recommended, SCDM uses the highest value. If no temperature is specified for all water solubility measurements for a substance, SCDM uses the highest value.

If water solubility values are not available in PHYSPROP, values are obtained from the references listed above, in the order they are listed. If no water solubility values are available in any of the first six references listed, or if the referenced value is suspect, a new value may be either selected from a data source outside the hierarchy or estimated. For any given substance, suspect values are identified by comparison with other water solubility values in SCDM data sources or other sources of chemical property data. The procedures described in Lyman *et al*. (1990) are used to estimate water solubility. RTI (1996) describes the use of these procedures for specific hazardous substances found in SCDM.

For the 49 volatile substances listed in Section 1.0 of this methodology document, only the PHYSPROP database was needed to obtain water solubility values.

2.3.3.2 Water Solubility - Metals and Metalloids

SCDM obtains water solubility values for metals and metalloid compounds from the following references, listed in order of priority:

- PHYSPROP Database. 2010. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.syrres.com/what-we-do/databaseforms.aspx?id=386. Accessed February 2012.
- CRC Handbook of Chemistry and Physics, 92nd Edition. June 2011. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.
- Lange's Handbook of Chemistry. 16th Edition. 2004, Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.
- Perry's Chemical Engineers' Handbook, 8th Edition. 2008, Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

If water solubility values are not available in PHYSPROP, values are obtained from the reference listed above, in the order they are listed. If values are not available from the first four references, SCDM determines and contains the geometric mean water solubility values for metals and metalloids as defined in the HRS (see HRS Section 3.2.1.2, Mobility) as the geometric mean of the highest and lowest water solubility values available for any inorganic compound containing the metal or metalloid.

For the 49 volatile substances listed in Section 1.0 of this methodology document, only the PHYSPROP database was needed to obtain water solubility values for metals and metalloids (i.e., mercury).

2.3.4 Soil/Water Distribution Coefficient (K_d); Soil Organic/Carbon Partition Coefficients (K_{OC} and Log K_{OW})

The soil/water distribution coefficient (K_d) values are used to calculate ground water mobility for hazardous substances that do not meet observed release criteria. If K_d values are not available, associated K_{OC} and Log K_{OW} values are used. All hazardous substances that are available to migrate from sources at the site to ground water are evaluated for ground water mobility. For organic substances, SCDM obtains K_d values from the EPA's Soil Screening Guidance (1996). If not available from the Soil Screening Guidance (http://www.epa.gov/superfund/health/conmedia/soil/index.htm), SCDM calculates the K_d according to HRS Section 3.2.1.2 (Mobility) and the relationship of $K_d = K_{OC} \times f_S$, where f_S is the sorbent content (fraction of

clays plus organic carbon) and K_{oc} is obtained from the following references, listed in order of priority:

- The Estimation Programs Interface (EPI) Suite™ (estimated values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/opptintr/exposure/pubs/episuite.htm. Accessed February 2012.

- U.S. EPA. 2002. Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites (Peer Review Draft), OSWER 9355.4-24. http://www.epa.gov/superfund/health/conmedia/soil/pdfs/ssg_main.pdf. Accessed February 2012.

- Yaws' Handbook of Thermodynamic and Physical Properties of Chemical Compounds. Knovel. http://www.knovel.com.

- The Estimation Programs Interface (EPI) Suite™ (experimental values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/opptintr/exposure/pubs/episuite.htm.

- Di'Toro, D.M. 1985. A Particle Interaction Model of Reversible Organic Chemical Sorption. Chemosphere. 14(10):1503-1538.

- Estimation procedures set forth by Lyman *et al*. 1990. Handbook of Chemical Property Estimation Methods. American Chemical Society, Washington, DC, as described in Research Triangle Institute (RTI). 1996. Chemical Properties for SCDM Development, Prepared for the U.S. EPA Office of Emergency and Remedial Response.

When using values from EPI Suite™, SCDM prefers K_{oc} values that are estimated using the Molecular Connectivity Index (MCI) method over K_{oc} values that are estimated by the Log K_{ow} method. When a K_{oc} is not available using the MCI method, SCDM uses the EPI Suite™ K_{oc} values estimated using the Log K_{ow} method. Information regarding collection of Log K_{ow} values is provided in Section 2.5.2 of this methodology document. Section 3.2 (Soil Water Distribution Coefficient [K_d]; Soil Organic/Carbon Partition Coefficients [K_{oc}]) of this document provides additional information regarding SCDM calculations of K_d and K_{oc} values. For 48 volatile organic substances listed in Section 1.0 of this methodology document, K_d values were not available from the EPA's Soil Screening Guidance. For these substances, K_d values were determined using MCI-estimated K_{oc} values obtained from EPI Suite™.

SCDM obtains soil/water distribution coefficient (K_d) values for metals from the following references, listed in order of priority:

- U.S. EPA. 2002. Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites (Peer Review Draft), Office of Solid Waste and Emergency Response. 9355.4-24. http://www.epa.gov/superfund/health/conmedia/soil/pdfs/ssg_main.pdf. Accessed February 2012.

- U.S. EPA. 1996. Soil Screening Guidance: Technical Background Document. EPA/540/R95/128. Office of Emergency and Remedial Response, Washington, DC. NTIS PB96-963502. http://www.epa.gov/superfund/health/conmedia/soil/index.htm. Accessed February 2012.

- Baes, C.F. III, R.D. Sharp, and A.L. Sjoreen, and R.W. Shor. 1984. A Review and Analysis of Parameters for Assessing Transportation of Environmentally Released Radionuclides through Agriculture. Oak Ridge

National Laboratory, TN. ORNL-5786.

- Di'Toro, D.M. 1985. A Particle Interaction Model of Reversible Organic Chemical Sorption. Chemosphere. 14(10):1503-1538.

SCDM contains values corresponding to typical subsurface pH (6.8). If K_d values are not available for metals in the EPA's Soil Screening Guidance, values are obtained from the references listed above, in the order they are listed. Of the 49 volatile substances listed in Section 1.0 of this methodology document, only mercury is a metal/metalloid substance. A K_d value for mercury was obtained from the EPA's Supplemental Guidance for Developing Soil Screening Levels for Superfund Sites.

2.4 Persistence Information

The evaluation of persistence is based primarily on the half-life of hazardous substances in surface water and secondarily on the sorption of the hazardous substances to sediments. Persistence information is used to determine the surface water persistence factor.

2.4.1 Hydrolysis, Biodegradation and Photolysis Half-Lives

SCDM obtains values for hydrolysis, biodegradation and photolysis half-lives from the following references, listed in order of priority:

- CHEMFATE Database. 2008. SRC. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.srcinc.com/what-we-do/databaseforms.aspx?id=381. Accessed February 2012.

- Handbook of Environmental Degradation Rates (HEDR). 1991. Howard, Phillip H., W.F. Jarvis, W.M. Meylan and E.M. Michalenko, Lewis Publishers, Inc. Chelsea, Michigan.

SCDM only uses values that have been measured in water from the CHEMFATE database. SCDM uses a value measured at 25°C. If more than one value measured at 25°C is available, SCDM uses the highest value. If no value is available at 25°C, a value determined at a temperature closest to 25°C is selected. If no temperature is specified for all half-life values for a substance, SCDM uses the highest value. If values are obtained from HEDR, SCDM uses only values listed as "first-order." If multiple values are provided, the highest value is used.

2.4.2 Volatilization Half-Lives

SCDM estimates volatilzation half-lives for organic substances in both rivers and lakes, using the equations and procedures described in Section 3.1 of this methodology document. Volatilization half-lives for metals and metalloids are obtained from the following reference:

- The Estimation Programs Interface (EPI) Suite™ (estimated values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/opptintr/exposure/pubs/episuite.htm. Accessed February 2012.

2.5 Bioaccumulation Potential Information

Bioconcentration factor (BCF) values for freshwater and saltwater (one set each for the human food chain threat and the environmental threat) are used to determine bioaccumulation potential factor values (40 CFR Part 300,

Appendix A, Section 4.1.3.2.1.3). If BCF data are not available for organic substances, the Log K_{OW} is used. Water solubility data are used if the Log K_{OW} exceeds 6.0, the substance is inorganic, or there is no Log K_{OW}.

2.5.1 Bioconcentration

Bioconcentration factor (BCF) values for freshwater and saltwater are used to determine the human food chain threat BCF and the environmental threat BCF. The BCF values in SCDM are preferentially based on actual measurements of bioconcentration in aquatic organisms. SCDM used BCF values from the following sources (listed in order of preference):

- U.S. EPA. 2012. ECOTOX Database. Environmental Research Laboratory, Duluth, MN. http://www.epa.gov/ecotox. Accessed February 2012.

- Versar, Inc. 1990. Issue Paper: Bioaccumulation Potential Based on Ambient Water Quality Criteria Documents (VER_BCF). Prepared for U.S. EPA Office of Emergency and Remedial Response, Washington, DC. Contract No. 68-W8-0098.

In SCDM, the highest measured value from ECOTOX is used. Measured values are preferred over calculated or estimated values. The above listed Versar reference is a report of a literature survey of BCF values developed for the purpose of obtaining preliminary values for use when the initial HRS was being developed. When using data from this reference, SCDM also prefers the highest measured value to an estimated value.

Environmental Threat: For the environmental threat, the highest value from any aquatic organism, regardless if it is consumed by humans, in each reference is used to establish environmental threat BCF values.

Human Food Chain Threat: The highest measured value from aquatic organisms typically known to be consumed by humans in each reference is used to establish the human food chain threat BCF values. Nonhuman food chain aquatic organisms are not used for the food chain BCF. Table 2 includes a list of some of the organisms for which BCF values may be taken. This list is intended to serve only as a guide to the SCDM data collector and hence, not all human food chain aquatic organisms are listed. Values from organisms not in this list may be used provided they are known to be consumed by humans.

Table 3. Examples of Human Food Chain Aquatic Organisms

American or Virginia oyster	Channel catfish	Lake whitefish	Rock bass
Asiatic clam	Clam	Mangrove snapper	Sauger
Atlantic salmon	Common bay mussel	Manila littleneck clam	Shore crab
Atlantic silverside	Common mirror colored carp	Mussel	Spot
Black bullhead	Common shrimp	Northern anchovy	Striped bass
Black crappie	Crayfish	Northern pike	Striped mullet
Black mussel	Dungeness or edible crab	Pilchard sardine	Swan mussel
Blue crab	Giant gourami	Pinfish	Tong sole
Bluegill	Gulf toadfish	Pink salmon	Topmouth gudgeon (golden shiner)
Brook trout	Kiyi	Rainbow trout	White mullet
Brown trout	Lake trout (siscowet)	Red swamp crayfish	White sand mussel

2.5.2 Octanol/Water Partition Coefficient (Log K_{OW})

Log K_{OW} values are used to determine the bioaccumulation potential factor value for a hazardous substance for which bioconcentration factor (BCF) data are not available. SCDM may also use the log K_{OW} to estimate a log K_{OC} when a K_{OC} is not available (see Section 3.2 of this methodology document). SCDM obtains n-octanol/water (log K_{OW}, also referred to as Log P) values from the following sources, listed in order of priority:

- The Estimation Programs Interface (EPI) Suite™ (experimental values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/opptintr/exposure/pubs/episuite.htm. Accessed February 2012.

- PHYSPROP Database. 2010. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.syrres.com/what-we-do/databaseforms.aspx?id=386. Accessed February 2012.

- CHEMFATE Database. 2008. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.srcinc.com/what-we-do/databaseforms.aspx?id=381. Accessed February 2012.

- CRC Handbook of Chemistry and Physics, 92nd Edition. June 2011. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.

- Research Triangle Institute (RTI). 1996. Chemical Properties for SCDM Development. Prepared for the U.S. EPA Office of Emergency and Remedial Response, Washington, DC.

The above references are listed in the preferential hierarchy for SCDM. While most of the hazardous substances in SCDM are addressed in RTI (1996), more recent data sources are preferred. If the more recent sources do not have data for specific substances, then the RTI (1996) reference is used. SCDM uses experimental values; estimated or calculated values are not used. If values are obtained from CHEMFATE, the recommended values are used. For the 49 volatile substances listed in Section 1.0 of this methodology document, EPI Suite™ experimental values were available for all substances except vinyl chloride; a log K_{OW} for vinyl chloride was obtained from the CHEMFATE database.

2.5.3 Water Solubility

Water solubility values are used to assign a bioaccumulation potential factor value for hazardous substances when BCF or log K_{OW} data are not available. See Sections 2.3.3.1 (Water Solubility - Nonmetallic Compounds) and 2.3.3.2 (Water Solubility - Metals and Metalloids) of this methodology document for the data collection protocol and guidance on water solubility values.

2.6 Ecotoxicity Parameters

Ecotoxicity data are used in the HRS scoring system to determine the Ecotoxicity Factor values (HRS; 40 CFR Part 300, Appendix A, Section 4.1.4.2.1.1). SCDM uses acute and chronic freshwater and saltwater criteria, and only uses those values specifically stated as criteria. If criteria are not available, then LC_{50} data are used.

2.6.1 Acute and Chronic Freshwater and Saltwater Criteria - CCC, CMC

The HRS (Section 4.1.4.2.1.1, Ecosystem Toxicity) uses the EPA Ambient Water Quality Criteria (AWQC) and

Ambient Aquatic Life Advisory Concentrations (AALAC) for assigning ecosystem toxicity factor values. The acute and chronic AWQC have been replaced by a new set of criteria, and the AALAC values do not exist. The new criteria replacing the AWQC for both freshwater and saltwater, are labeled as (1) Criteria Maximum Concentration (CMC), to be used in place of what was previously acute AWQC, and (2) Criteria Continuous Concentration (CCC), to be used in place of what was previously chronic AWQC. These new values closely correspond to the old acute and chronic AWQC values, respectively; however, some values have been re-derived using different methodology and, therefore, the resulting values must be used as directed by the EPA. Many of the CMC and CCC values have associated endnotes regarding how the value was derived and how it should be used. SCDM also contains these endnotes. Some CMC and CCC values are baseline values that must be adjusted using the information specified in the endnotes. The CMC and CCC values are taken from:

- U.S. EPA. 2012. National Recommended Water Quality Criteria - 2002. Office of Water. Washington, DC. http://water.epa.gov/scitech/swguidance/standards/current/index.cfm#altable. Accessed February 2012.

2.6.2 LC_{50} - Freshwater, Saltwater

SCDM obtains LC_{50} data from the ECOTOX database, for both freshwater and saltwater.

- U.S. EPA. 2012. ECOTOX Database. Environmental Research Laboratory, Duluth, MN. http://www.epa.gov/ecotox. Accessed February 2012.

SCDM uses the lowest acute LC_{50} value found for any aquatic organism in the specified environment with an acute exposure duration of ≥1 day and ≤ 4 days. When no durations or environments are given, LC_{50} values are not entered into SCDM.

2.7 Regulatory Benchmarks

The HRS assigns extra weight to targets with exposure to hazardous substances at levels that are at or above regulatory benchmark values. This section describes the sources for regulatory limits that the HRS uses as health-based or ecological-based benchmarks.

2.7.1 National Ambient Air Quality Standards (NAAQS)

National Ambient Air Quality Standards (NAAQS) are used to establish Level I concentrations. Targets exposed to concentrations at or above the NAAQS are scored as Level I targets. SCDM uses data from the following source to obtain NAAQS:

- 40 CFR Part 50. 2010. National Ambient Air Quality Standards. http://www.epa.gov/air/criteria.html. Accessed February 2012.

2.7.2 National Emissions Standards for Hazardous Air Pollutants (NESHAPs)

National Emission Standards for Hazardous Air Pollutants (NESHAPs) are used to establish Level I concentrations. Targets exposed to concentrations at or above NESHAPs are scored as Level I targets. SCDM uses data from the following source to obtain NESHAPs, and uses only those values that are reported in ambient concentration units ($\mu g/m^3$):

- 40 CFR Part 61 and Part 63. 2011. National Emission Standards for Hazardous Air Pollutants. http://www.epa.gov/compliance/monitoring/programs/caa/neshaps.html. Accessed February 2012.

2.7.3 Maximum Contaminant Levels (MCLs) and Maximum Contaminant Level Goals (MCLGs)

Maximum Contaminant Levels (MCLs) and Maximum Contaminant Level Goals (MCLGs) are used to establish Level I concentrations. Targets exposed to concentrations at or above MCLs and MCLGs are scored as Level I targets. SCDM uses data from the following sources for MCLs and MCLGs:

- U.S. EPA. 2009. National Primary Drinking Water Standards. Accessed through List of Drinking Water Contaminants and MCLs. Office of Water, Washington, DC. http://water.epa.gov/drink/contaminants/index.cfm. Accessed February 2012.

- U.S. EPA. 2000e. Soil Screening Guidance for Radionuclides: User's Guide (EPA/540-R-00-007, PB2000 963307). http://www.epa.gov/superfund/health/contaminants/radiation/radssg.htm. Accessed February 2012.

SCDM uses only MCLs that are reported in units of concentration (mg/L, µg/L or pCi/L) and only non-zero MCLGs that are reported in units of concentration (mg/L or µ/L). For substances where multiple values are listed, SCDM uses the lowest number. For substances where both MCLs and MCLGs are reported but are different, SCDM selects the lower of the two values.

2.7.4 FDA Action Levels (FDAALs)

Food and Drug Administration Action Levels (FDAAL) are used to establish Level I concentrations. Targets exposed to concentrations at or above FDAALs are scored as Level I targets. SCDM contains FDAALs for fish and shellfish only, and obtains the FDAAL values from the following reference:

- U.S. Food and Drug Administration. 2000. Action Levels for Poisonous or Deleterious Substances in Human and Animal Feed. Center for Food Safety and Applied Nutrition, Washington, D.C. http://www.fda.gov/Food/GuidanceComplianceRegulatoryInformation/GuidanceDocuments/ChemicalContaminantsandPesticides/ucm077969.htm. Accessed February 2012.

2.7.5 Ecological Based Benchmarks

See Section 2.6.1 of this document for information regarding acute Criteria Maximum Concentration (CMC) and chronic Criteria Continuous Concentration (CCC) for freshwater and saltwater.

2.8 Physical Properties

SCDM contains hazardous substance physical property data including, but not limited to, chemical formula, molecular weight, density, boiling point and melting point. SCDM applies yes/no flags to classify physical property data into the four substance categories defined below.

Organic Substances ("Organic"): "Y" indicates that the substance is organic, and "N" indicates an inorganic substance. This flag is used to determine factor values for ground water mobility and bioaccumulation potential. Volatile and semivolatile organics are indicated. These flags influence the SCDM calculation of K_d values.

Metal-Containing Substances ("Metal Contain"): "Y" indicates that the substance is a metal or metalloid or an inorganic compound that contains a metal or metalloid. "N" indicates that the substance is not, or does not contain, a metal or metalloid. This flag is used to determine factor values for ground water mobility and surface water persistence.

Radioactive Isotope ("Radionuclide"): "Y" indicates that the substance is a specific radioactive isotope, and "N" indicates that it is not. In SCDM, a substance cannot be both a radioactive element and a specific radioactive isotope. This flag is used to determine factor values for human toxicity, ecosystem toxicity and surface water persistence.

Radioactive Element ("Rad. Element"): "Y" indicates that the substance is a radioactive element, and "N" indicates that it is not. In SCDM, a substance cannot be both a radioactive element and a specific radioactive isotope. This flag determines whether or not the HRS factors and benchmarks are printed in Appendix A.

2.8.1 Chemical Formula, Boiling Point and Melting Point

Chemical formula, boiling point and melting point data are extracted directly from the following sources, in order of priority:

- PHYSPROP Database. 2010. Syracuse Research Corporation (SRC). Syracuse, NY. http://www.syrres.com/what-we-do/databaseforms.aspx?id=386. Accessed February 2012.
- CRC Handbook of Chemistry and Physics, 92nd Edition. June 2011. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.
- The Estimation Programs Interface (EPI) Suite™ (experimental values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/opptintr/exposure/pubs/episuite.htm. Accessed February 2012.
- Perry's Chemical Engineers' Handbook, 8th Edition. 2008, Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

2.8.2 Molecular Weight

Molecular weight data are collected from the following sources, in order of priority:

- The Estimation Programs Interface (EPI) Suite™ (experimental values) developed by the U.S. Environmental Protection Agency's Office of Pollution Prevention and Toxics and Syracuse Research Corporation (SRC). http://www.epa.gov/opptintr/exposure/pubs/episuite.htm. Accessed February 2012.
- CRC Handbook of Chemistry and Physics, 92nd Edition. June 2011. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.
- Perry's Chemical Engineers' Handbook, 8th Edition. 2008, Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.
- Lange's Handbook of Chemistry. 16th Edition. 2004, Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.
- Yaws' Handbook of Thermodynamic and Physical Properties of Chemical Compounds. Knovel. http://www.knovel.com. Accessed February 2012.

2.8.3 Density

Density data are collected from the following sources, in order of priority:

- CRC Handbook of Chemistry and Physics, 92nd Edition. June 2011. W.M. Haynes, National Institute of Standards and Technology, CRC Press, Boulder, Colorado. ISBN-10: 1439855110/ISBN-13: 978-1439855119.

- Perry's Chemical Engineers' Handbook, 8th Edition. 2008, Perry, Roberts H., Green, Don W., McGraw-Hill, ISBN: 978-0-07-142294-9.

- Lange's Handbook of Chemistry. 16th Edition. 2004, Speight, James G., McGraw-Hill, ISBN-10:0071432205 / ISBN-13: 978-0071432207.

3.0 CALCULATIONS IN SCDM

3.1 Volatilization Half-Life

SCDM estimates the volatilization half-life in surface water for organic substances using Equation 1 (presented as Equation 15-12 in Thomas, R.G. in the "Handbook of Chemical Property and Estimation Methods," Lyman, *et al*.[1] In this method, the volatilization half-life ($T_{1/2}$) can be expressed as follows:

$$T_{1/2} = \left[\frac{Z \times \ln 2}{K_L \text{ hr}} \right] \quad (1)$$

Where:
Z = Mean water body depth (cm)
K_L = Overall liquid-phase mass transfer coefficient.

The following expression gives the overall liquid-phase mass transfer coefficient:

$$K_L = \frac{(H/RT)k_g \times k_l}{(H/RT)k_g + k_l} \text{ cm/hr} \quad (2)$$

Where:
H = Henry's Law constant ($atm \cdot m^3/mol$)
R = Universal gas constant (8.2×10^{-5} $atm \cdot m^3/mol \cdot K$)
T = Temperature (K; ºC + 273)
k_g = Gas-phase exchange coefficient
k_l = Liquid-phase exchange coefficient

The gas-phase exchange coefficient expression depends on the molecular weight (MW) of the compound.

- If molecular weight (MW) is <65 g/mol, the following equation is used:

$$k_g = 3{,}000 \times (18 / MW)^{1/2} \text{ cm/hr} \quad (3)$$

- If MW is ≥65 g/mol, the following equation is used:

$$k_g = 1{,}137.5 \times (V_{wind} + V_{curr})(18 / MW)^{1/2} \text{ cm/hr} \quad (4)$$

Where:
V_{wind} = Wind velocity (m/sec)
V_{curr} = Current velocity (m/sec)

The liquid-phase exchange coefficient expression also depends on the molecular weight of the compound.

[1] Thomas, R.G. 1990. "Volatilization from Water." In Handbook of Chemical Property Estimation Methods. W.J. Lyman, W.F. Reehl, D.H. Rosenblatt, Eds. American Chemical Society, Washington, DC, 15:9–28. 0-ISBN 8412-1761-0.

- If MW is <65 g/mol, the following equation is used:

$$k_l = 20 \times (44 / MW)^{1/2} \text{ cm/hr} \quad (5)$$

- If MW is ≥65 g/mol, the expression also depends on the wind and current velocities; the following equation is used when V_{wind} is ≤1.9 m/sec and MW is ≥65 g/mol:

$$k_l = 23.51 \times (V_{curr}^{0.969} / Z^{0.673}) \times (32 / MW)^{1/2} \text{ cm/hr} \quad (6)$$

The following equation is used when V_{wind} is >1.9 m/sec and ≤5 m/sec, and MW is ≥65 g/mol:

$$k_l = 23.51 \times (V_{curr}^{0.969} / Z^{0.673}) \times (32 / MW)^{1/2} e^{0.526(V_{wind} - 1.9)} \text{cm/hr} \quad (7)$$

No liquid-phase exchange coefficient equation is provided in Thomas (1990) for wind velocities >5 m/sec.

Combining Equations (1), (2), (3), and (5) into a single equation for estimating volatilization half-life ($T_{1/2}$) for compounds with MW <65 g/mol gives the following equation:

$$T_{1/2} = Z \times \ln 2 \times \{[(1/20) \times (MW/44)^{1/2}] + [(RT/H \times 3000) \times (MW/18)^{1/2}]\} \text{ hr} \quad (8)$$

The following equation, combining Equations (1), (2), (4), and (6), can be used to estimate the volatilization half-life ($T_{1/2}$) for compounds with MW ≥65 g/mol if the wind velocity is ≤1.9 m/sec:

$$T_{1/2} = Z \times \ln 2 \times \{[(Z^{0.673} / 23.51 \times V_{curr}^{0.969}) \times (MW/32)^{1/2}] + [(RT/H \times 1{,}137.5) \times (V_{wind} + V_{curr}) \times (MW/18)^{1/2}]\} \text{ hr} \quad (9)$$

The following equation, combining Equations (1), (2), (4), and (7), can be used to estimate the volatilization half-life ($T_{1/2}$) for compounds with MW ≥65 g/mol if the wind velocity is >1.9 m/sec and ≤5 m/sec:

$$T_{1/2} = Z \times \ln 2 \times \{[(Z^{0.673} / 23.51 \times V_{curr}^{0.969}) \times (MW/32)^{1/2}] e^{0.526(1.9 - V_{wind})} + [(RT/H \times 1{,}137.5) \times (V_{wind} + V_{curr}) \times (MW/18)^{1/2}]\} \text{ hr} \quad (10)$$

If H is $<10^{-7}$ atm·m^3/mol, the substance is less volatile than water and its concentration will increase as the water evaporates. The substance is considered essentially nonvolatile (Thomas, 1990, p. 15-15) and no volatilization half-life is estimated for rivers or lakes.

3.1.1 Volatilization Half-Life for Rivers, Oceans, Coastal Tidal Waters and the Great Lakes

To calculate the volatilization half-life for rivers, oceans, coastal tidal waters and the Great Lakes, the mean water body depth is taken as 100 cm, the temperature as 298 K, the wind velocity as 0.5 m/sec and the current velocity as 1 m/sec. Using these values, Equations (8) and (10) reduce to the following:

- If MW <65 g/mol:

$$T_{1/2} = 2.89 \times \{[0.05 \times (MW/44)^{1/2}] + [(8.1 \times 10^{-6}/H) \times (MW/18)^{1/2}]\} \text{ days} \quad (11)$$

- If MW ≥65 g/mol:

$$T_{1/2} = 2.89 \times \{[0.185 \times (MW/32)^{1/2}] + [(3.6 \times 10^{-6}/H) \times (MW/18)^{1/2}]\} \text{ days} \quad (12)$$

Where:
H = Henry's Law Constant (atm·m^3/mol)
MW = Molecular Weight (g/mol)

3.1.2 Volatilization Half-Life for Lakes

To calculate the volatilization half-life for lakes, the mean water body depth is taken as 100 cm, the temperature as 298 K, the wind velocity as 0.5 m/sec and the current velocity as 0.05 m/sec. Using these values, Equations (8) and (9) reduce to the following:

- If MW <65 g/mol:

$$T_{1/2} = 2.89 \times \{[0.05 \times (MW/44)^{1/2}] + [(8.1 \times 10^{-6}/H) \times (MW/18)^{1/2}]\} \text{ days} \quad (13)$$

- If MW ≥65 g/mol:

$$T_{1/2} = 2.89 \times \{[17.2 \times (MW/32)^{1/2}] + [(3.9 \times 10^{-6}/H) \times (MW/18)^{1/2}]\} \text{ days} \quad (14)$$

Where:
H = Henry's Law Constant (atm·m^3/mol)
MW = Molecular Weight (g/mol)

3.2 Soil Water Distribution Coefficient (K_d); Soil Organic/Carbon Partition Coefficients (K_{oc})

In the evaluation of the ground water migration pathway, a hazardous substance that does not meet the criteria for an observed release is assigned a mobility factor value from HRS Table 3-8 (Ground Water Mobility Factor Values) based on its K_d value and its water solubility value. K_d values that are not available in the references listed in Section 2.3.4 of this methodology document are calculated as detailed below:

HRS Section 3.2.1.2 (Mobility) states:

> For any hazardous substance that does not meet the criteria for an observed release by chemical analysis to at least one of the aquifers, assign that hazardous substance a mobility factor value from Table 3-8 for the aquifer being evaluated, based on its water solubility and distribution coefficient (K_d)…….. For any hazardous substance that is organic and that does not meet the criteria for an observed release by chemical analysis, establish a distribution coefficient for that hazardous substance as follows:

Estimate K_d range for the hazardous substance using the following equation:

$$K_d = (K_{oc})(f_s) \quad (15)$$

Where:
K_{oc} = Soil-water partition coefficient for organic carbon for the hazardous substance
f_s = Sorbent content (fraction of clays plus organic carbon) in the subsurface

- Use f_s values of 0.03 and 0.77 in the above equation to establish the upper and lower values of the K_d range for the hazardous substance.
- Calculate the geometric mean of the upper and lower K_d range values. Use this geometric mean as the distribution coefficient in assigning the hazardous substance a mobility factor value from [HRS] Table 3-8.

When a K_{oc} is not available to calculate K_d values, SCDM uses the Log P or Log K_{ow} to estimate K_{oc} values. To perform this calculation, SCDM uses the relationship determined by Di'Toro (1985) for semivolatile organic compounds:

$$\text{Log } K_{oc} = 0.00028 + (0.983 \text{ Log } K_{ow}) \quad (16)$$

For volatile organic compounds, chlorinated benzenes, and certain chlorinated pesticides, SCDM uses the relationship derived in the Soil Screening Guidance Technical Background Document (EPA, 1996):

$$\text{Log } K_{oc} = 0.00784 + (0.7919 \text{ Log } K_{ow}) \quad (17)$$

3.3 Screening Concentration Benchmarks

Section 3.3 details the equations and exposure assumptions that are used to determine screening concentration benchmarks for the subset of 49 volatile substances contained in SCDM. The sources and determination of the substance-specific values used in these equations are detailed in Section 2.0 of this methodology document.

3.3.1 Screening Concentration Benchmarks for the Air Migration Pathway

The following equations are used to determine air inhalation screening concentration benchmarks for the air migration pathway. The benchmarks use exposure parameters and factors that represent Reasonable Maximum Exposure (RME) conditions for long-term/chronic exposures and are based on the methodology outlined in the EPA's *Risk Assessment Guidance for Superfund, Part B* (1991) and *Risk Assessment Guidance for Superfund, Part F* (2009). General equations are provided for volatile compounds in Section 3.3.1.1 (non-carcinogenic benchmarks) and Section 3.3.1.2 (carcinogenic benchmarks). Equations that are specific for substances that are carcinogenic through a mutagenic mode of action, including vinyl chloride and trichloroethylene (TCE), are provided in Section 3.3.1.3.

3.3.1.1 Non-carcinogenic – Air, Inhalation

$$SC_{nc-air} = \frac{THQ \times (AT \times ED) \times \left(\frac{1000\ \mu g}{mg}\right)}{EF \times ED \times ET \times \left(\frac{1\ day}{24\ hours}\right) \times \frac{1}{RfC}} \quad (18)$$

<u>*Where*</u>:
SC_{nc-air} = Air Inhalation Screening Concentration, Non-Carcinogenic (µg/m^3)
THQ = Target hazard quotient (=1), unitless
AT = Averaging time (365 days/year)
ED = Exposure duration (30 years)
EF = Exposure frequency (350 days/year)
ET = Exposure time (24 hours/day)
RfC = Inhalation reference concentration (mg/m^3)

Using the exposure assumptions listed above, Equation (18) can be simplified as:

$$SC_{nc-air} = 1042.857 \times RfC \quad (19)$$

3.3.1.2 Carcinogenic – Air, Inhalation

$$SC_{c-air} = \frac{TR \times (AT \times LT)}{EF \times ED \times ET \times \left(\frac{1\ day}{24\ hours}\right) \times IUR} \quad (20)$$

<u>*Where*</u>:
SC_{c-air} = Air Inhalation Screening Concentration, Carcinogenic (µg/m^3)
TR = Target risk (1 x 10^{-6}) (unitless)
AT = Averaging time (365 days/year)
LT = Lifetime (70 years)

ED = Exposure duration (30 years)
EF = Exposure frequency (350 days/year)
ET = Exposure time (24 hours/day)
IUR = Inhalation unit risk $(\mu g/m^3)^{-1}$

Using the exposure assumptions listed above, Equation (20) can be simplified as:

$$SC_{c-air} = \frac{2.433 \times 10^{-6}}{IUR} \tag{21}$$

3.3.1.3 Carcinogenic through a Mutagenic Mode of Action – Air, Inhalation

$$SC_{mu-air} = \frac{TR \times (AT \times LT)}{EF \times ET \times \left(\frac{1\ day}{24\ hours}\right) \times [(ED_{0-2} \times IUR \times 10) + (ED_{2-6} \times IUR \times 3) + (ED_{6-16} \times IUR \times 3) + (ED_{16-30} \times IUR \times 1)]} \tag{22}$$

<u>*Where*</u>:
$SC_{mu\text{-}air}$ = Air Inhalation Screening Concentration, Carcinogenic – Mutagenic Mode of Action $(\mu g/m^3)$
TR = Target risk (1 x 10^{-6}) (unitless)
AT = Averaging time (365 days/year)
LT = Lifetime (70 years)
$ED_{0\text{-}2}$ = Exposure duration (2 years)
$ED_{2\text{-}6}$ = Exposure duration (4 years)
$ED_{6\text{-}16}$ = Exposure duration (10 years)
$ED_{16\text{-}30}$ = Exposure duration (14 years)
EF = Exposure frequency (350 days/year)
ET = Exposure time (24 hours/day)
IUR = Inhalation unit risk $(\mu g/m^3)^{-1}$

Using the exposure assumptions listed above, Equation (22) can be simplified as:

$$SC_{mu-air} = \frac{9.605 \times 10^{-7}}{IUR} \tag{23}$$

3.3.1.3.1 Vinyl Chloride – Air, Inhalation

$$SC_{mu-vc} = \frac{TR}{IUR + \left[\frac{IUR \times EF \times ED \times ET \times (1\ day / 24\ hours)}{(AT \times LT)}\right]} \tag{24}$$

<u>*Where*</u>:
$SC_{mu\text{-}vc}$ = Air Inhalation Screening Concentration, Vinyl Chloride $(\mu g/m^3)$
TR = Target risk (1 x 10^{-6})
AT = Averaging time (365 days/year)
LT = Lifetime (70 years)
ED = Exposure duration (30 years)
EF = Exposure frequency (350 days/year)

ET = Exposure time (24 hours/day)
IUR = Inhalation unit risk $(\mu g/m^3)^{-1}$

Using the exposure assumptions listed above, Equation (24) can be simplified as:

$$SC_{mu-vc} = \frac{7.090 \times 10^{-7}}{IUR} \quad (25)$$

3.3.1.3.2 Trichloroethylene – Air, Inhalation

The following three steps are used to calculate an air inhalation cancer screening concentration benchmark for TCE.

Step 1. A mutagenic screening concentration (SC) is calculated using the kidney IUR and the mutagenic equation provided below.

$$SC_{mu-tce} = \frac{TR \times (AT \times LT)}{EF \times ET \times (1\ day / 24\ hours) \times [(ED_{0-2} \times IUR \times 10) + (ED_{2-6} \times IUR \times 3) + (ED_{6-16} \times IUR \times 3) + (ED_{16-30} \times IUR \times 1)]} \quad (26)$$

Where:
$SC_{mu\text{-}tce}$ = Air Inhalation Screening Concentration, Carcinogenic–Mutagenic Mode of Action $(\mu g/m^3)$
TR = Target risk (1×10^{-6}) (unitless)
AT = Averaging time (365 days/year)
LT = Lifetime (70 years)
$ED_{0\text{-}2}$ = Exposure duration (2 years)
$ED_{2\text{-}6}$ = Exposure duration (4 years)
$ED_{6\text{-}16}$ = Exposure duration (10 years)
$ED_{16\text{-}30}$ = Exposure duration (14 years)
EF = Exposure frequency (350 days/year)
ET = Exposure time (24 hours/day)
IUR = Inhalation unit risk $(\mu g/m^3)^{-1}$

Using the exposure assumptions listed above, Equation (26) can be simplified as:

$$SC_{mu-tce} = \frac{0.0256}{350 \times [(20 \times IUR) + (12 \times IUR) + (30 \times IUR) + (14 \times IUR)]} \quad (27)$$

Step 2. A cancer SC is calculated using the non-Hodgkin's lymphoma (NHL) and liver cancer IUR and the cancer equation provided below.

$$SC_{c-tce} = \frac{TR \times (AT \times LT)}{EF \times ED \times ET \times (1\ day / 24\ hours) \times IUR} \quad (28)$$

Where:
$SC_{c\text{-}tce}$ = Air Inhalation Screening Concentration, Carcinogenic $(\mu g/m^3)$
TR = Target risk (1×10^{-6}) (unitless)
AT = Averaging time (365 days/year)
LT = Lifetime (70 years)

ED = Exposure duration (30 years)
EF = Exposure frequency (350 days/year)
ET = Exposure time (24 hours/day)
IUR = Inhalation unit risk $(\mu g/m^3)^{-1}$

Using the exposure assumptions listed above, Equation (28) can be simplified as:

$$SC_{c-tce} \quad \frac{0.0256}{10{,}500 \times IUR} \tag{29}$$

Step 3. A cumulative result of both the mutagenic and cancer screening concentrations calculated in Steps 1 and 2 above is then generated, and the resulting value reflects both the kidney cancer risk (mutagenic risk estimate) and the NHL and liver cancer risk.

$$SC_{mu-c-tce} = \frac{1}{\left(\frac{1}{SC_{m-air}}\right) + \left(\frac{1}{SC_{c-air}}\right)} \tag{30}$$

3.3.2 Screening Concentration Benchmarks for the Soil Exposure Pathway

The following equations are used to determine soil ingestion screening concentration benchmarks for the soil exposure pathway. The benchmarks use exposure parameters and factors that represent RME conditions for long-term/chronic exposures and are based on the methodology outlined in the EPA's *Risk Assessment Guidance for Superfund, Part B* (1991). General equations are provided for volatile compounds in Section 3.3.2.1 (non-carcinogenic benchmarks) and Section 3.3.2.2 (carcinogenic benchmarks). Equations that are specific for substances that are carcinogenic through a mutagenic mode of action, including vinyl chloride and TCE, are provided in Section 3.3.2.3.

3.3.2.1 Non-carcinogenic – Soil, Ingestion

$$SC_{res\text{-}sol\text{-}nc\text{-}ing} = \frac{THQ \times AT \times ED_C \times BW_C}{EF \times ED_C \times \left(\frac{1}{RfD}\right) \times IRS_C \times \frac{10^{-6}\,kg}{mg}} \tag{31}$$

Where:
$SC_{res\text{-}sol\text{-}nc\text{-}ing}$ = Soil Screening Concentration, Non-Carcinogenic (mg/kg)
RfD = Oral reference dose (in mg/kg-day)
AT = Averaging time – resident (365 days/year)
BW_c = Body weight – child (= 15 kg)
ED_c = Exposure duration – resident child (= 6 years)
EF = Exposure frequency – resident (= 350 days/year)
IRS_c = Resident soil ingestion rate – child (= 200 mg/day)
THQ = Target hazard quotient (=1)

Using the exposure assumptions listed above, Equation (31) can be simplified as:

$$SC_{res-sol-nc-ing} = 78214.29 \times RfD \tag{32}$$

3.3.2.2 Carcinogenic – Soil, Ingestion

$$SC_{res-sol-ca-ing} = \frac{TR \times AT \times LT}{SF \times EF \times IFS \times \frac{10^{-6}\,kg}{mg}} \quad (33)$$

Where:
$SC_{res\text{-}sol\text{-}ca\text{-}ing}$ = Soil Screening Concentration, Carcinogenic (mg/kg)
IFS = Soil ingestion rate – resident, age adjusted [= (114 mg-year) / (kg-day)], calculated as:

$$= \left(\frac{EDc \times IRS_c}{BW_c} \right) + \left[\frac{(ED_r - ED_C) \times IRS_a}{BW_a} \right]$$

SF = Chronic oral cancer slope factor $(mg/kg\text{-}day)^{-1}$
TR = Target risk (= 1×10^{-6})
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
ED_c = Exposure duration – resident child (= 6 years)
ED_r = Exposure duration – resident (= 30 years)
IRS_a = Resident soil ingestion rate – adult (= 100 mg/day)
IRS_c = Resident soil ingestion rate – child (= 200 mg/day)
BW_a = Body weight – adult (= 70 kg)
BW_c = Body weight – child (= 15 kg)

Using the exposure assumptions listed above, Equation (33) can be simplified as:

$$SC_{res-sol-ca-ing} = \frac{0.64}{SF} \quad (34)$$

3.3.2.3 Carcinogenic through a Mutagenic Mode of Action – Soil, Ingestion

$$SC_{res-sol-mu-ing} = \frac{TR \times AT \times LT}{SF \times EF \times IFSM \times \frac{10^{-6}\,kg}{mg}} \quad (35)$$

Where:
$SC_{res\text{-}sol\text{-}mu\text{-}ing}$ = Soil Screening Concentration, Carcinogenic – Mutagenic Mode of Action (mg/kg)
IFSM = Mutagenic soil ingestion rate – resident, age adjusted [= (489.5 mg-year) / (kg-day)], calculated as:

$$= \left(\frac{ED_{0-2} \times IRS_c \times 10}{BW_c} \right) + \left(\frac{ED_{2-6} \times IRS_c \times 3}{BW_c} \right) + \left(\frac{ED_{6-16} \times IRS_a \times 3}{BW_a} \right) + \left(\frac{ED_{16-30} \times IRS_a \times 1}{BW_a} \right)$$

SF = Chronic oral cancer slope factor $(mg/kg\text{-}day)^{-1}$
TR = Target risk (= 1×10^{-6})
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
$ED_{0\text{-}2}$ = Exposure duration – resident ages 0-2 (= 2 years)

$ED_{2\text{-}6}$ = Exposure duration – resident ages 2-6 (= 4 years)
$ED_{6\text{-}16}$ = Exposure duration – resident ages 6-16 (= 10 years)
$ED_{16\text{-}30}$ = Exposure duration – resident ages 16-30 (= 14 years)
IRS_a = Resident soil ingestion rate – adult (= 100 mg/day)
IRS_c = Resident soil ingestion rate – child (= 200 mg/day)
BW_a = Body weight – adult (= 70 kg)
BW_c = Body weight – child (= 15 kg)

Using the exposure assumptions listed above, Equation (35) can be simplified as:

$$SC_{res\text{-}sol\text{-}mu\text{-}ing} = \frac{0.149}{SF} \tag{36}$$

3.3.2.3.1 Vinyl Chloride – Soil, Ingestion

$$SC_{res\text{-}sol\text{-}ca\text{-}vc\text{-}ing} = \frac{TR}{\left[\left(\frac{SF \times EF \times IFS \times \frac{10^{-6}\,kg}{mg}}{AT \times LT}\right) + \left(\frac{SF \times IRS_C \times \frac{10^{-6}\,kg}{mg}}{BW_C}\right)\right]} \tag{37}$$

<u>*Where*</u>:
$SC_{res\text{-}sol\text{-}ca\text{-}vc\text{-}ing}$ = Soil Screening Concentration, Vinyl Chloride (mg/kg)
IFS = Soil ingestion rate – resident, age adjusted [= (114 mg-year) / (kg-day)], calculated as:

$$= \left(\frac{EDc \times IRS_c}{BW_c}\right) + \left[\frac{(ED_r - ED_c) \times IRS_a}{BW_a}\right]$$

SF = Chronic oral cancer slope factor $(mg/kg\text{-}day)^{-1}$
TR = Target risk ($= 1 \times 10^{-6}$)
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
ED_c = Exposure duration – child (= 6 years)
ED_r = Exposure duration – resident (= 30 years)
IRS_a = Resident soil ingestion rate – adult (= 100 mg/day)
IRS_c = Resident soil ingestion rate – child (= 200 mg/day)
BW_a = Body weight – adult (= 70 kg)
BW_c = Body weight – child (= 15 kg)

Using the exposure assumptions listed above, Equation (37) can be simplified as:

$$SC_{res\text{-}sol\text{-}ca\text{-}vc\text{-}ing} = \frac{0.067}{SF} \tag{38}$$

3.3.2.3.2 Trichloroethylene (TCE) – Soil, Ingestion

The following three steps were used to calculate a soil screening concentration benchmark reflecting exposure only via ingestion.

Step 1. A mutagenic screening concentration (SC) is calculated using the kidney cancer slope factor and the mutagenic equation provided below.

$$SC_{sol\text{-}mu\text{-}tce\text{-}ing} = \frac{TR \times AT \times LT}{SF \times EF \times IFSM \times \frac{10^{-6}\,kg}{mg}} \quad (39)$$

Where:

$SC_{\text{-}sol\text{-}mu\text{-}tce\text{-}ing}$ = Soil Screening Concentration, Mutagenic (mg/kg)

$IFSM$ = Mutagenic soil ingestion rate–resident, age adjusted [=(489.5 mg-year)/(kg-day)], calculated as:

$$= \left(\frac{ED_{0-2} \times IRS_c \times 10}{BW_c}\right) + \left(\frac{ED_{2-6} \times IRS_c \times 3}{BW_c}\right) + \left(\frac{ED_{6-16} \times IRS_a \times 3}{BW_a}\right) + \left(\frac{ED_{16-30} \times IRS_a \times 1}{BW_a}\right)$$

SF = Chronic oral slope factor $(mg/kg\text{-}day)^{-1}$
TR = Target risk (= 1×10^{-6})
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
$ED_{0\text{-}2}$ = Exposure duration – resident ages 0-2 (= 2 years)
$ED_{2\text{-}6}$ = Exposure duration – resident ages 2-6 (= 4 years)
$ED_{6\text{-}16}$ = Exposure duration – resident ages 6-16 (= 10 years)
$ED_{16\text{-}30}$ = Exposure duration – resident ages 16-30 (= 14 years)
IRS_a = Resident soil ingestion rate – adult (= 100 mg/day)
IRS_c = Resident soil ingestion rate – child (= 200 mg/day)
BW_a = Body weight – adult (= 70 kg)
BW_c = Body weight – child (= 15 kg)

Using the exposure assumptions listed above, Equation (39) can be simplified as:

$$SC_{soil\text{-}mu\text{-}tce\text{-}ing} = \frac{0.02555}{SF \times 0.1713} \quad (40)$$

Step 2. A cancer screening concentration (SC) is calculated using the NHL and liver cancer slope factor and the cancer equation provided below.

$$SC_{sol\text{-}ca\text{-}tce\text{-}ing} = \frac{TR \times AT \times LT}{SF \times EF \times IFS \times \frac{10^{-6}\,kg}{mg}} \quad (41)$$

Where:

$SC_{\text{-}sol\text{-}ca\text{-}tce\text{-}ing}$ = Soil Screening Concentration, Carcinogenic (mg/kg)
IFS = Soil ingestion rate – resident, age adjusted [= (114 mg-year) / (kg-day)], calculated as:

$$= \left(\frac{EDc \times IRS_c}{BW_c}\right) + \left[\frac{(ED_r - ED_C) \times IRS_a}{BW_a}\right]$$

SF = Chronic oral cancer slope factor $(mg/kg\text{-}day)^{-1}$

TR = Target risk (= 1 x 10^{-6})
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
ED_c = Exposure duration – child (= 6 years)
ED_r = Exposure duration – resident (= 30 years)
IRS_a = Resident soil ingestion rate – adult (= 100 mg/day)
IRS_c = Resident soil ingestion rate – child (= 200 mg/day)
BW_a = Body weight – adult (= 70 kg)
BW_c = Body weight – child (= 15 kg)

Using the exposure assumptions listed above, Equation (41) can be simplified as:

$$SC_{soil\text{-}ca\text{-}tce-ing} = \frac{0.02555}{SF \times 0.0399} \tag{42}$$

Step 3. A cumulative result of both the mutagenic and cancer screening concentrations, via oral ingestion, calculated in Steps 1 and 2 above is then generated and the resulting value reflects both the kidney cancer risk (mutagenic risk estimate) and the NHL and liver cancer risk.

$$SC_{soll-ca-mu-tce-ing} = \frac{1}{\left(\frac{1}{SC_{soil\text{-}ca\text{-}ing}}\right) + \left(\frac{1}{SC_{soil\text{-}mu\text{-}ing}}\right)} \tag{43}$$

3.3.3 Screening Concentration Benchmarks for the Ground Water and Drinking Water Pathways

The following equations are used to determine water ingestion screening concentration benchmarks. The benchmarks use exposure parameters and factors that represent RME conditions for long-term/chronic exposures and are based on the methodology outlined in the EPA's *Risk Assessment Guidance for Superfund, Part B* (1991). General equations are provided for volatile compounds in Section 3.3.3.1 (non-carcinogenic benchmarks) and Section 3.3.3.2 (carcinogenic benchmarks). Equations that are specific for substances that are carcinogenic through a mutagenic mode of action, including vinyl chloride and TCE, are provided in Section 3.3.3.3.

3.3.3.1 Non-carcinogenic – Ground Water and Drinking Water, Ingestion

$$SC_{water\text{-}nc\text{-}ing} = \frac{THQ \times AT \times ED_C \times BW_C \times 1000}{EF \times ED_C \times \left(\frac{1}{RfD}\right) \times IRW_C} \tag{44}$$

Where:
$SC_{water\text{-}nc\text{-}ing}$ = Ground Water/Drinking Water Screening Concentration, Non-Carcinogenic (µg/L)
RfD = Oral reference dose (in mg/kg-day)
AT = Averaging time – resident (365 days/year)
BW_c = Body weight – child (= 15 kg)
ED_c = Exposure duration – child (= 6 years)
EF = Exposure frequency – resident (= 350 days/year)

IRW_c = Drinking water ingestion rate – resident child (= 1 L/day)
THQ = Target hazard quotient (=1)

Using the exposure assumptions listed above, Equation (44) can be simplified as:

$$SC_{water\text{-}nc\text{-}ing} = 15642.86 \times RfD \quad (45)$$

3.3.3.2 Carcinogenic – Ground Water and Drinking Water, Ingestion

$$SC_{water\text{-}ca\text{-}ing} = \frac{TR \times AT \times LT \times 1000}{SF \times EF \times IFW} \quad (46)$$

Where:
$SC_{water\text{-}ca\text{-}ing}$ = Ground Water/Drinking Water Screening Concentration, Carcinogenic (µg/L)

IFW = Drinking water ingestion rate – Resident, adjusted [= (1.086 L-year) / (kg-day)], calculated as:

$$= \left(\frac{ED_C \times IRW_c}{BW_c} \right) + \left[\frac{(ED_r - ED_C) \times IRW_a}{BW_a} \right]$$

SF = Chronic oral slope factor $(mg/kg\text{-}day)^{-1}$
TR = Target risk ($= 1 \times 10^{-6}$)
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
ED_c = Exposure duration – child (= 6 years)
ED_r = Exposure duration – resident (= 30 years)
IRW_a = Drinking water ingestion rate – resident adult (= 2 L/day)
IRW_c = Drinking water ingestion rate – resident child (= 1 L/day)
BW_a = Body weight – adult (= 70 kg)
BW_c = Body weight – child (= 15 kg)

Using the exposure assumptions listed above, Equation (46) can be simplified as:

$$SC_{water\text{-}ca\text{-}ing} = \frac{0.0672}{SF} \quad (47)$$

3.3.3.3 Carcinogenic through a Mutagenic Mode of Action – Ground Water and Drinking Water, Ingestion

$$SC_{water\text{-}mu\text{-}ing} = \frac{TR \times AT \times LT \times 1000}{SF \times EF \times IFWM} \quad (48)$$

Where:
$SC_{water\text{-}mu\text{-}ing}$ = Ground Water/Drinking Water Screening Concentration, Mutagenic (µg/L)
$IFWM$ = Mutagenic Drinking Water ingestion rate – resident, age adjusted [= (3.39 L-year) / (kg-day)], calculated as:

$$= \left(\frac{ED_{0-2} \times IRW_c \times 10}{BW_c} \right) + \left(\frac{ED_{2-6} \times IRW_c \times 3}{BW_c} \right) + \left(\frac{ED_{6-16} \times IRW_a \times 3}{BW_a} \right) + \left(\frac{ED_{16-30} \times IRW_a \times 1}{BW_a} \right)$$

SF = Chronic oral slope factor (mg/kg-day)$^{-1}$
TR = Target risk (= 1 x 10^{-6})
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
$ED_{0\text{-}2}$ = Exposure duration – resident ages 0-2 (= 2 years)
$ED_{2\text{-}6}$ = Exposure duration – resident ages 2-6 (= 4 years)
$ED_{6\text{-}16}$ = Exposure duration – resident ages 6-16 (= 10 years)
$ED_{16\text{-}30}$ = Exposure duration – resident ages 16-30 (= 14 years)
IRW_a = Drinking water ingestion rate – resident adult (= 2 L/day)
IRW_c = Drinking water ingestion rate – resident child (= 1 L/day)
BW_a = Body weight – adult (= 70 kg)
BW_c = Body weight – child (= 15 kg)

Using the exposure assumptions listed above, Equation (48) can be simplified as:

$$SC_{water\text{-}mu\text{-}ing} = \frac{0.0215}{SF} \tag{49}$$

3.3.3.3.1 Vinyl Chloride – Ground Water and Drinking Water, Ingestion

$$SC_{res\text{-}water\text{-}ca\text{-}vc\text{-}ing} = \frac{TR}{\left[\left(\frac{SF \times EF \times IFW \times \frac{mg}{1000\ \mu g}}{AT \times LT}\right) + \left(\frac{SF \times IRW_C \times \frac{mg}{1000\ \mu g}}{BW_C}\right)\right]} \tag{50}$$

Where:
$SC_{res\text{-}water\text{-}nc\text{-}ing}$ = Ground Water/Drinking Water Screening Concentration, Vinyl Chloride (µg/L)
IFW = Drinking water ingestion rate – Resident, adjusted [= (1.086 L-year) / (kg-day)], calculated as:

$$= \left(\frac{ED_C \times IRW_C}{BW_C}\right) + \left[\frac{(ED_R - ED_C) \times IRW_a}{BW_a}\right]$$

SF = Chronic oral slope factor (mg/kg-day)$^{-1}$
TR = Target risk (= 1 x 10^{-6})
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
ED_c = Exposure duration –child (= 6 years)
ED_r = Exposure duration – resident (= 30 years)
IRW_a = Drinking water ingestion rate – resident adult (= 2 L/day)
IRW_c = Drinking water ingestion rate – resident child (= 1 L/day)
BW_a = Body weight – adult (= 70 kg)
BW_c = Body weight – child (= 15 kg)

Using the exposure assumptions listed above, Equation (50) can be simplified as:

$$SC_{res\text{-}water\text{-}ca\text{-}vc\text{-}ing} = \frac{0.0123}{SF} \tag{51}$$

3.3.3.3.2 Trichloroethylene (TCE) – Ground Water and Drinking Water, Ingestion

The following three steps were used to calculate a drinking water screening concentration reflecting exposure only via ingestion.

Step 1. A mutagenic screening concentration (SC) is calculated using the kidney cancer slope factor and the equation provided below.

$$SC_{water\text{-}mu\text{-}tce-ing} = \frac{TR \times AT \times LT \times 1000}{SF \times EF \times IFWM} \quad (52)$$

Where:

$SC_{water\text{-}mu\text{-}tce\text{-}ing}$ = Drinking Water Screening Concentration, Mutagenic Mode of Action (µg/L)

$IFWM$ = Mutagenic Drinking Water ingestion rate – resident, age adjusted [= (3.39 L-year) / (kg-day)], calculated as:

$$= \left(\frac{ED_{0-2} \times IRW_c \times 10}{BW_c}\right) + \left(\frac{ED_{2-6} \times IRW_c \times 3}{BW_c}\right) + \left(\frac{ED_{6-16} \times IRW_a \times 3}{BW_a}\right) + \left(\frac{ED_{16-30} \times IRW_a \times 1}{BW_a}\right)$$

SF = Chronic oral cancer slope factor $(mg/kg\text{-}day)^{-1}$

TR = Target risk $(= 1 \times 10^{-6})$

AT = Averaging time – resident (= 365 days/year)

LT = Lifetime (= 70 years)

EF = Exposure frequency – resident (= 350 days/year)

$ED_{0\text{-}2}$ = Exposure duration – resident ages 0-2 (= 2 years)

$ED_{2\text{-}6}$ = Exposure duration – resident ages 2-6 (= 4 years)

$ED_{6\text{-}16}$ = Exposure duration – resident ages 6-16 (= 10 years)

$ED_{16\text{-}30}$ = Exposure duration – resident ages 16-30 (= 14 years)

IRW_a = Drinking water ingestion rate – resident adult (= 2 L/day)

IRW_c = Drinking water ingestion rate – resident child (= 1 L/day)

BW_a = Body weight – adult (= 70 kg)

BW_c = Body weight – child (= 15 kg)

Using the exposure assumptions listed above, Equation (52) can be simplified as:

$$SC_{water\text{-}mu-tce\text{-}ing} = \frac{25.55}{SF \times 1186.5} \quad (53)$$

Step 2. A cancer SC is calculated using the NHL and liver cancer slope factor and equation provided below.

$$SC_{water\text{-}ca\text{-}tce-ing} = \frac{TR \times AT \times LT \times 1000}{SF \times EF \times IFW} \quad (54)$$

Where:

$SC_{water\text{-}ca\text{-}tce\text{-}ing}$ = Drinking Water Screening Concentration, Carcinogenic (µg/L)

IFW = Drinking water ingestion rate – Resident, adjusted [= (1.086 L-year) / (kg-day)], calculated as:

$$= \left(\frac{ED_C \times IRW_c}{BW_c}\right) + \left[\frac{(ED_r - ED_C) \times IRW_a}{BW_a}\right]$$

SF = Chronic oral cancer slope factor $(mg/kg\text{-}day)^{-1}$

TR = Target risk $(= 1 \times 10^{-6})$

AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
EF = Exposure frequency – resident (= 350 days/year)
ED_c = Exposure duration – child (= 6 years)
ED_r = Exposure duration – resident (30 years)
IRW_a = Drinking water ingestion rate – resident adult (= 2 L/day)
IRW_c = Drinking water ingestion rate – resident child (= 1 L/day)
BW_a = Body weight – adult (= 70 kg)
BW_c = Body weight – child (= 15 kg)

Using the exposure assumptions listed above, Equation (54) can be simplified as:

$$SC_{water\text{-}ca\text{-}tce\text{-}ing} = \frac{25.55}{SF \times 380.1} \tag{55}$$

Step 3. A cumulative result of both the oral mutagenic and oral cancer screening concentrations calculated in Steps 1 and 2 above is then generated and the resulting value reflects both the kidney cancer risk (mutagenic risk estimate) and NHL and liver cancer risk.

$$SC_{water\text{-}ca\text{-}mu\text{-}tce\text{-}ing} = \frac{1}{\left(\frac{1}{SC_{water\text{-}ca\text{-}ing}}\right) + \left(\frac{1}{SC_{water\text{-}mu\text{-}ing}}\right)} \tag{56}$$

3.3.4 Screening Concentration Benchmarks for the Human Food Chain Pathway

The following equations are used to determine screening concentration benchmarks for the human food chain exposure pathway. The benchmarks use exposure parameters and factors that represent RME conditions for long-term/chronic exposures and are based on the methodology outlined in the EPA's *Risk Assessment Guidance for Superfund, Part B* (1991). General equations are provided for volatile compounds in Section 3.3.4.1 (non-carcinogenic benchmarks) and Section 3.3.4.2 (carcinogenic benchmarks). Equations that are specific for substances that are carcinogenic through a mutagenic mode of action, including vinyl chloride and TCE, are provided in Section 3.3.1.3.

3.3.4.1 Non-carcinogenic – Human Food Chain, Fish Ingestion

$$SC_{res\text{-}fsh\text{-}nc\text{-}ing} = \frac{THQ \times AT \times ED_r \times BW_a}{EF \times ED_r \times \left(\frac{1}{RfD}\right) \times IRF \times \frac{10^{-6}\,kg}{mg}} \tag{57}$$

Where:
$SC_{res\text{-}fsh\text{-}nc\text{-}ing}$ = Human Food Chain Screening Concentration, Fish Ingestion, Non-Carcinogenic (mg/kg)
RfD = Oral reference dose (in mg/kg-day)
AT = Averaging time – resident (365 days/year)
BW_a = Body weight – adult (= 70 kg)
ED_r = Exposure duration – resident (= 30 years)
EF = Exposure frequency – resident (= 350 days/year)
IRF = Fish ingestion rate (= 5.4 x 10^4 mg / day)
THQ = Target hazard quotient (=1)

Using the exposure assumptions listed above, Equation (57) can be simplified as:

$$SC_{res\text{-}fsh\text{-}nc\text{-}ing} = 1351.85 \times RfD \tag{58}$$

3.3.4.2 Carcinogenic – Human Food Chain, Fish Ingestion

$$SC_{res-fsh\text{-}ca\text{-}ing} = \frac{TR \times AT \times LT \times BW_a}{EF \times ED_r \times SF \times IRF \times \frac{10^{-6}\,kg}{mg}} \tag{59}$$

Where:
$SC_{res\text{-}fsh\text{-}ca\text{-}ing}$ = Human Food Chain Screening Concentration, Fish Ingestion, Carcinogenic (mg/kg)
SF = Chronic oral cancer slope factor $(mg/kg\text{-}day)^{-1}$
TR = Target risk (= 1×10^{-6})
AT = Averaging time – resident (= 365 days/year)
LT = Lifetime (= 70 years)
BW_a = Body weight – adult (= 70 kg)
EF = Exposure frequency – resident (= 350 days/year)
ED = Exposure duration – resident (= 30 years)
IRF = Fish ingestion rate (= 5.4×10^4 mg / day)

Using the exposure assumptions listed above, Equation (59) can be simplified as:

$$SC_{res\text{-}fsh-ca\text{-}ing} = \frac{0.00315}{SF} \tag{60}$$

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